

## Structural Characterization of Dental Glasses by Multinuclear Solid State NMR

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The so called “dental” glasses have been widely used in the field of dentistry due to their ability to generate (after adequate heat treatment) glass-ceramics having appropriate chemical and mechanical properties.<sup>1-3</sup> A range of glasses with attractive properties and synthesized by newer methods have been developed in the last years and studied by solid state NMR spectroscopy. Owing to its element-selective, inherently quantitative character and sensitivity to local environments, this technique is ideally suited for structural studies of multicomponent glasses.<sup>1</sup> In this work, some “dental” silicate glasses containing several network modifiers, network formers and intermediates at different compositions, have been characterized by solid state magic angle spinning (MAS)-NMR spectroscopy for the <sup>29</sup>Si, <sup>31</sup>P and <sup>27</sup>Al nuclei. Preliminary results revealed the presence of two-, three- and four-fold coordinated silicon species with minor fractions of four-coordinate species present in the samples. The fractional contribution of the Si<sup>(3)</sup> and Si<sup>(4)</sup> sites is significantly higher in the glass containing the higher amount of SiO<sub>2</sub>. In contrast, <sup>31</sup>P MAS-NMR spectra reveal that phosphorous is almost exclusively present in the form of depolymerized orthophosphate species (P<sup>(0)</sup>) in all investigated glasses. Small amounts of P<sup>(1)</sup> units are also present, whose fraction decreases with the increase of SiO<sub>2</sub> content. <sup>27</sup>Al MAS NMR spectra for the samples containing different amounts of Al<sub>2</sub>O<sub>3</sub> show the presence of dominantly four-coordinated aluminum species (signal centered near 50 ppm). Small amounts of five- and six-fold coordinated aluminum species are also present, as indicated by the signals near 20 and -10 ppm, respectively. The largest fraction of higher-coordinated aluminum is present in sample having the highest Al content (2.61 mole% of <sup>27</sup>Al). The resonance shifts observed for Al<sup>(5)</sup> and Al<sup>(6)</sup> appear at lower values than usually observed in peraluminous aluminosilicate glasses. The preliminary results reveal initial insights about the structural speciation of these complex glasses and instigate the continuity of the investigation in terms of the study of the local environment of other NMR-relevant nuclei, as well as in the investigation of the short- and medium-range order and heteroatomic connectivities of a mixed-network former glass system to unprecedented detail by employing modern NMR techniques.

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